

Variational Wavefunction for the Periodic Anderson Model with Onsite Correlation Factors

Katsunori Kubo and Hiroaki Onishi

Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan

We propose a variational wavefunction containing parameters to tune the probabilities of all the possible onsite configurations for the periodic Anderson model. We call it the full onsite-correlation wavefunction (FOWF). This is a simple extension of the Gutzwiller wavefunction (GWF), in which one parameter is included to tune the double occupancy of the f electrons at the same site. We compare the energy of the GWF and the FOWF evaluated by the variational Monte Carlo method and that obtained with the density-matrix renormalization group method. We find that the energy is considerably improved in the FOWF. On the other hand, the physical quantities do not change significantly between these two wavefunctions as long as they describe the same phase, such as the paramagnetic phase. From these results, we not only demonstrate the improvement by the FOWF, but we also gain insights on the applicability and limitation of the GWF to the periodic Anderson model.

In solid states, the Coulomb interaction between electrons reduces or renormalizes the energy scale for the electrons. An extreme example of such an electron correlation effect is the heavy-fermion phenomenon. In heavy-fermion systems, the effective mass of the electrons, which is proportional to the inverse of the energy scale, can become a thousand times larger than the bare electron mass. Then, exotic order such as unconventional superconductivity has been found, in particular, in the vicinity of the quantum critical points of heavy-fermion materials.

As a canonical model for the heavy-fermion phenomenon, the periodic Anderson model has been employed, which is composed of conduction and f electrons, and the effects of the Coulomb interaction between f electrons have been studied by various methods. In particular, theories based on a variational wavefunction called the Gutzwiller wavefunction (GWF) have succeeded in describing the heavy-fermion state.¹⁻⁴ In the GWF, one parameter, called the Gutzwiller parameter, is introduced to tune the probability of the double occupancy of f electrons on the same site. The above theories assumed the paramagnetic (PM) state; however, within the GWF, it has also been revealed that the PM state is unstable against magnetic order in the parameter region where the heavy-fermion state is realized.^{1,3,5-11}

To overcome this difficulty, we should improve the variational wavefunction. For this purpose, it is useful to consult the literature on other multiorbital systems since the periodic Anderson model is also a multiorbital system with the conduction band and f orbital. For multiorbital Hubbard models, parameters that tune the probabilities of all the possible onsite configurations have been introduced.^{12,13} Here, we call this type of wavefunction the

full onsite-correlation wavefunction (FOWF). The variational Monte Carlo method has been applied to the FOWF to evaluate the energy and physical quantities in the multiorbital Hubbard models.¹⁴⁻¹⁶

It is natural to use the FOWF for the multiorbital Hubbard models since all the orbitals are subjected to the Coulomb interactions. On the other hand, in the periodic Anderson model, it seems to be sufficient to consider the GWF at first glance since the Coulomb interaction acts only on the electrons in the f orbital. However, the antiferromagnetic correlation between the conduction and f electrons is also important in the periodic Anderson model. Actually, it results in the Kondo phenomena and the Ruderman-Kittel-Kasuya-Yosida interaction, which have been central issues in condensed matter physics. Thus, it would be a natural improvement to consider all the possible onsite correlations, including the spin-dependent correlations between the conduction and f electrons, in addition to the f - f correlation.

In this paper, we consider the FOWF for the periodic Anderson model and apply the variational Monte Carlo method.² As a benchmark of the wavefunction, we study the model on a one-dimensional chain and compare the energy with that obtained with the density-matrix renormalization group (DMRG) method.¹⁷ Then, we discuss how much the energy is improved from the GWF. We also compare physical quantities evaluated by the GWF and by the FOWF. In this paper, we not only emphasize the improvement by the FOWF, but also note the situations where the GWF is still useful by comparing the results between these two wavefunctions.

The periodic Anderson model is given by

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i\sigma} \epsilon_f n_{fi\sigma} - V \sum_{k\sigma} (f_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_{k\sigma}) + U \sum_i n_{fi\uparrow} n_{fi\downarrow}, \quad (1)$$

where $c_{k\sigma}^\dagger$ and $f_{k\sigma}^\dagger$ are the creation operators of the conduction and f electrons, respectively, with momentum k and spin σ , and $n_{fi\sigma}$ is the number operator of the f electron with spin σ at site i . ϵ_k is the kinetic energy of the conduction electron, ϵ_f is the energy level of the f orbital, V is the hybridization matrix element between the conduction and f electrons, and U is the onsite Coulomb interaction for the f orbital. The Coulomb interaction U is large since the spatial extent of the f -orbital wavefunction is narrow. In this study, we simply take $U \rightarrow \infty$ since we will obtain qualitatively the same results even for a finite U as long as it is sufficiently large, for example, comparable to the band width of the conduction electrons, to describe f -electron compounds. Actually, within the GWF, we have obtained qualitatively similar results for a finite U .¹¹ For the kinetic energy of the conduction electrons, we consider only the nearest-neighbor hopping on a one-dimensional chain, and it is given by $\epsilon_k = -2t \cos k$, where t is the hopping integral and we set the lattice constant as unity.

We apply the variational Monte Carlo method to the model.² We consider two types of wavefunction as mentioned in the introductory part.

One is the GWF, which has been used to study this model, for example, by the variational Monte Carlo method as in this study.^{2,8,9,11} For $U \rightarrow \infty$, the Gutzwiller parameter is zero, and the GWF is given by

$$|\psi_G\rangle = P_G |\phi\rangle, \quad (2)$$

where

$$P_G = \prod_i [1 - n_{fi\uparrow} n_{fi\downarrow}]. \quad (3)$$

The projection operator P_G excludes the double occupancy of the f electrons at the same site. $|\phi\rangle$ is the one-electron part of the wavefunction. We define it as the ground state of a mean-field-type effective Hamiltonian, which we will give later.

The other variational wavefunction is the FOWF. It is defined as

$$|\psi_{FO}\rangle = P_{FO} |\phi\rangle, \quad (4)$$

where

$$P_{FO} = \prod_{\gamma i} [1 - (1 - g_\gamma) P_{\gamma i}], \quad (5)$$

with $P_{\gamma i} = |\gamma i\rangle \langle \gamma i|$, which is the projection operator to state γ at site i . $|\phi\rangle$ is the one-electron part as in the GWF. While this type of wavefunction has been used to

study multiorbital Hubbard models,^{12–16} it has not been applied to the periodic Anderson model. Since we consider one conduction band and one f orbital, there are 16 onsite states. By considering symmetry and conservation of the number of electrons for each spin, we can reduce the number of independent variational parameters that we have to optimize. In addition, for γ denoting a configuration with doubly occupied f electrons, $g_\gamma = 0$ since $U \rightarrow \infty$. The FOWF reduces to the GWF if we set $g_\gamma = 1$ for configurations γ without doubly occupied f electrons.

In this study, we consider the PM and ferromagnetic (FM) states, i.e., spatially uniform states. Then, the effective Hamiltonian is given by¹¹

$$H_{\text{eff}} = \sum_{k\sigma} (c_{k\sigma}^\dagger \ f_{k\sigma}^\dagger) \begin{pmatrix} \epsilon_k & -\tilde{V}_\sigma \\ -\tilde{V}_\sigma & \tilde{\epsilon}_{f\sigma} \end{pmatrix} \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix}, \quad (6)$$

where \tilde{V}_σ is the effective hybridization matrix element and $\tilde{\epsilon}_{f\sigma}$ is the effective f -level, which are also variational parameters. For the PM state, they do not depend on the spin σ . We diagonalize H_{eff} and construct its ground state $|\phi\rangle$ while fixing the electron number n_σ per site of each spin σ . In the PM state, $n_\uparrow = n_\downarrow$. For the FM state, the magnetization $M = n_\uparrow - n_\downarrow$ is a parameter characterizing the state.

For each state, we evaluate the energy by the Monte Carlo method and optimize the variational parameters that minimize the energy. For the FM state, we also have to optimize the magnetization. Then, we compare the energies of these states with the same electron density $n = n_\uparrow + n_\downarrow$ and determine the ground state. Other physical quantities can also be calculated by the Monte Carlo method with the optimized variational parameters.

In this study, we set $U \rightarrow \infty$, $V = t$, and $n = 1.25$. The calculations are carried out for a 40-site chain with a periodic boundary condition.

Figure 1 shows the energy E per site of the GWF and FOWF for the PM and FM states as functions of ϵ_f . The energy is measured from that of the GWF for the PM state $E_{\text{GWF PM}}$. The statistical errors are much smaller than the symbol sizes, and we do not draw them. In addition, we have also evaluated the energy by the DMRG method¹⁷ (stars in Fig. 1), by which we can accurately determine the ground state of a one-dimensional system as the present model in an unbiased manner. In the DMRG calculations, we have performed extrapolation to zero truncation error by using data for up to 800 DMRG states.

For both types of variational wavefunction, the energy for the PM and FM states coincides at higher values of ϵ_f , that is, the energy takes a minimum at $M = 0$ and the system is in the PM phase. At lower values of ϵ_f , the energy of the FM state becomes lower than that in the PM state, and the ground state is FM there. By the DMRG method, we obtained the PM state for $\epsilon_f/t = 0$

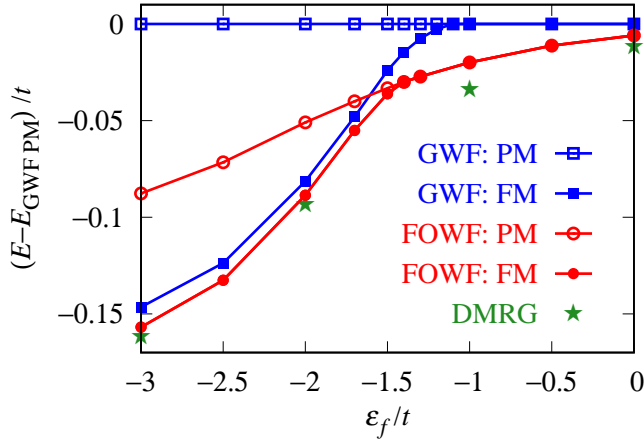


Fig. 1. (Color online) Energy as functions of ϵ_f measured from that of the Gutzwiller wavefunction (GWF) for the paramagnetic (PM) state $E_{\text{GWF PM}}$: the GWF (squares) and the full onsite-correlation wavefunction (FOWF, circles) for the PM state (open symbols) and for the ferromagnetic (FM) state (solid symbols). $U/t \rightarrow \infty$, $V/t = 1$, and $n = 1.25$. The energy obtained by the DMRG method for a sufficiently large value of the Coulomb interaction, $U/t = 1000$, is also shown (stars).

and -1 and the FM state for $\epsilon_f/t = -2$ and -3 .

In both the PM and FM phases, by improving the wavefunction from the GWF to the FOWF, the energy becomes very close to that of the DMRG method. In other words, by only including the onsite projection factors, we can greatly improve the energy. The FM transition point, where the FM energy departs from the PM energy, shifts to a lower value of ϵ_f , since more fluctuations are included in the FOWF in comparison with in the GWF, and the FM ordered state becomes unstable to a certain extent.

In principle, the order of the transition can be determined by the slope of E : it is second-order when the slope is continuous at the transition point and first-order when the slope is discontinuous. The order of the transition seems to be second-order in both the wavefunctions, while it is difficult to exclude the possibility of a weak first-order transition from the present numerical calculations on a finite-size lattice.

In Fig. 2, we show the FM moment as a function of ϵ_f . Note that the state with $M = 2 - n = 0.75$ is a half-metallic state, in which the Fermi surface for the up-spin electrons disappears. The magnetization seems to develop from zero continuously, which is consistent with the second-order transition suggested from the behavior of the energy. However, we mention again that we should investigate larger lattices carefully to determine the order of the transition since we have to deal with states with smaller values of magnetization, which require higher resolution. This is beyond the scope of the present study. The overall behavior of the magnetization is similar between the GWF and FOWF, but the

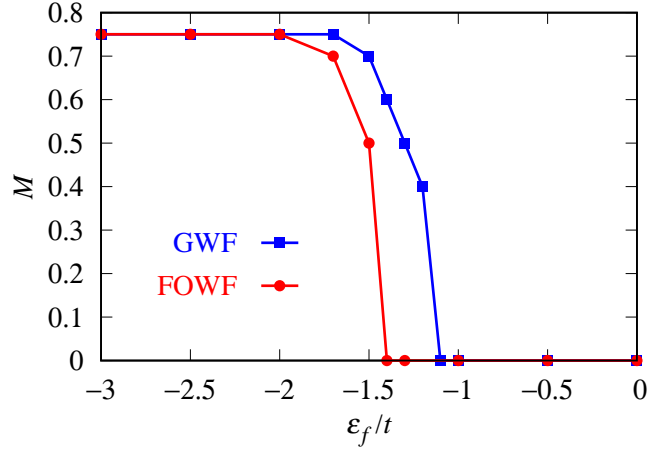


Fig. 2. (Color online) Magnetization for the GWF (squares) and FOWF (circles) as functions of ϵ_f . $U/t \rightarrow \infty$, $V/t = 1$, and $n = 1.25$.

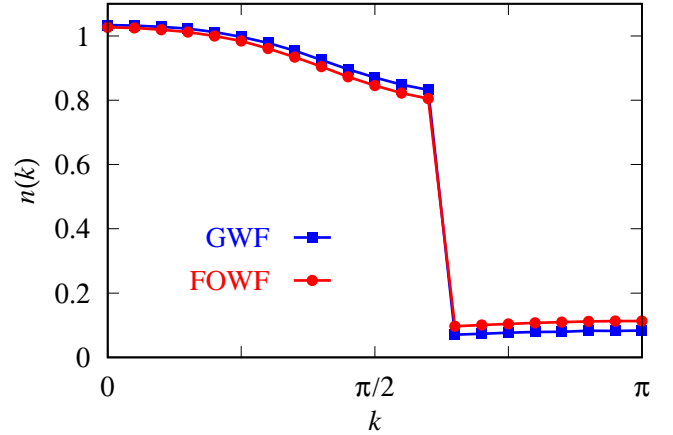


Fig. 3. (Color online) Momentum distribution functions in the PM phase of the GWF (squares) and FOWF (circles). $U/t \rightarrow \infty$, $V/t = 1$, $n = 1.25$, and $\epsilon_f/t = -1$.

FM transition point shifts to a lower value of ϵ_f in the FOWF as discussed above.

To investigate the electronic state further, we also calculate the momentum distribution function. The momentum distribution function is defined as

$$n_{\sigma}(k) = \langle c_{k\sigma}^{\dagger} c_{k\sigma} \rangle + \langle f_{k\sigma}^{\dagger} f_{k\sigma} \rangle, \quad (7)$$

where $\langle \dots \rangle$ denotes the expectation value. It does not depend on the spin σ in the PM state: $n_{\uparrow}(k) = n_{\downarrow}(k) = n(k)$. The momentum distribution functions of the GWF and FOWF are shown in Fig. 3 for $\epsilon_f/t = -1$ and in Fig. 4 for $\epsilon_f/t = -2$. Both wavefunctions result in the PM phase for $\epsilon_f/t = -1$ and in the FM phase for $\epsilon_f/t = -2$ (see Figs. 1 and 2). The slight but finite increase in $n(k)$ in Fig. 3 with k above the Fermi momentum is an artifact of the present wavefunctions without

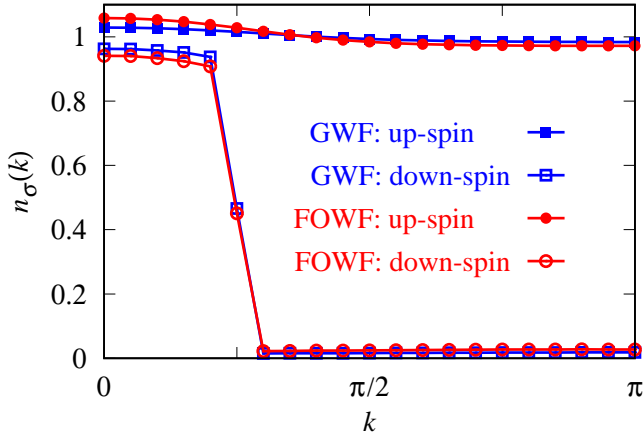


Fig. 4. (Color online) Momentum distribution functions in the FM phase of the GWF (squares) and FOWF (circles). Solid (open) symbols are for up-spin (down-spin) states. $U/t \rightarrow \infty$, $V/t = 1$, $n = 1.25$, and $\epsilon_f/t = -2$.

intersite correlations.^{2,18,19} $n_\downarrow(k)$ in Fig. 4 is also an increasing function above the Fermi momentum for the same reason, although it is invisible on this scale.

While the energy is significantly improved from the GWF to the FOWF, the momentum distribution functions are very similar between these wavefunctions. Thus, we expect that physical quantities can be evaluated accurately even by the GWF as long as both wavefunctions describe the same phase.

In one-dimensional correlated systems, we expect a Tomonaga–Luttinger liquid state in general. However, we see a clear jump in the momentum distribution function at the Fermi momentum in Figs. 3 and 4, indicating a Fermi liquid. This is due to the fact that we have used variational wavefunctions for Fermi liquid states. To describe a Tomonaga–Luttinger liquid state, we should carefully consider intersite correlations, which are not included here.^{20–22} In addition, the disappearance of the jump may be difficult to observe for a finite-size lattice as in this study, even if we improve the wavefunction further.

However, the size of the apparent jump may be used to measure the correlation effect, and conclusions extracted from this quantity should be applicable to higher-dimensional systems, where Fermi liquid states are expected. In other words, we expect that the characteristics of the variational wavefunctions considered here will not depend strongly on the dimensionality, although the applicability will depend strongly. If the correlation effect becomes strong, the size of the jump should be reduced. Actually, the jump is reduced slightly in the FOWF in comparison with in the GWF.

By using the jump $\Delta n_\sigma(k_F)$ at the Fermi momentum,

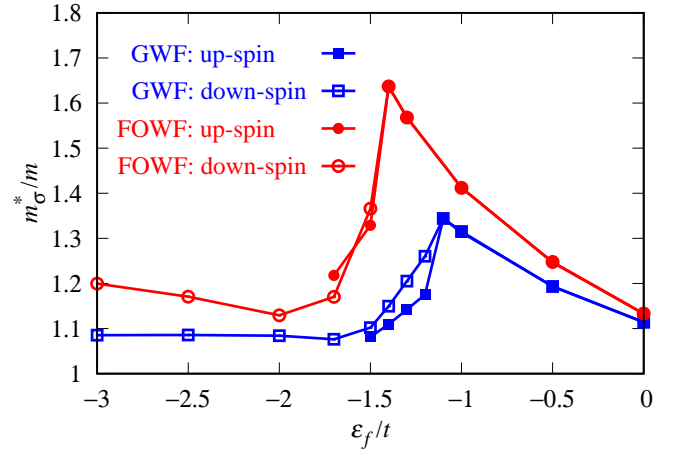


Fig. 5. (Color online) Effective mass as functions of ϵ_f of the GWF for up-spin (solid squares) and down-spin (open squares) electrons and of the FOWF for up-spin (solid circles) and down-spin (open circles) electrons. $U/t \rightarrow \infty$, $V/t = 1$, and $n = 1.25$.

we can define the effective mass m_σ^* as

$$\frac{m_\sigma^*}{m} = \frac{1}{\Delta n_\sigma(k_F)}, \quad (8)$$

where m is the bare electron mass. Figure 5 shows the ϵ_f dependence of the effective mass. Note that in the half-metallic state, we cannot define the effective mass for up-spin electrons since the Fermi surface disappears for them. While the effective mass is enhanced in the FOWF as expected, the overall behavior is similar between these wavefunctions. The main difference is the position of the FM transition. The PM phase extends to lower values of ϵ_f in the FOWF and, as a result, the FOWF can attain a larger effective mass. If we assume a PM state, we can obtain a large effective mass even in the GWF, and actually the heavy-fermion state has been discussed by using the GWF with this assumption.^{1–4} The present study provides a justification of this assumption of the PM state to some extent.

However, the obtained effective mass in the FOWF is still not very large. We have also evaluated the effective mass for $n = 1.75$ since the correlation effects become stronger near half-filling, $n = 2$. Actually, the effective mass at the same ϵ_f in the PM phase becomes larger, but the FM transition point shifts to a higher value of $\epsilon_f \simeq 1$ and we also do not obtain a very large effective mass in the PM phase for $n = 1.75$. Thus, to obtain a larger effective mass, we should further improve the wavefunction and/or revise the model if we take the possibility of magnetic order into consideration.

Concerning other quantities, such as the effective f -level $\tilde{\epsilon}_{f\sigma}$, the energy gain at the transition, and the contribution of the f electrons to $\Delta n_\sigma(k_F)$, the behaviors do not change significantly from those in the GWF, as the physical quantities explicitly presented in this paper.

See Refs. 10 and 11 for details of these quantities.

To summarize, we have proposed a wavefunction for the periodic Anderson model containing parameters to tune all the possible onsite configurations (we named it the FOWF) to improve the Gutzwiller wavefunction (GWF). Although the FOWF does not require a large computational effort since only the onsite variational parameters are included, the energy is considerably improved and becomes close to the value obtained with the density-matrix renormalization group method. However, physical quantities, such as the magnetization and the effective mass, do not change significantly between the GWF and FOWF as long as they are in the same phase. The main differences between these two wavefunctions appear in the energy and in the position of the FM transition point.

From these observations, we conclude that we can use the GWF to discuss the heavy-fermion state by assuming the PM state, since we can expect that the PM region will become wider when we improve the wavefunction, but the physical quantities can be evaluated accurately even by the GWF. However, to discuss the magnetic transition point itself and the behavior around it, such as quantum critical phenomena, it is better to use a wavefunction beyond the GWF.

Acknowledgments This work was supported by JSPS KAKENHI Grant Numbers JP15K05191 and JP16K05494. Part of the computations were carried out on the supercomputers at the Japan

Atomic Energy Agency and the Institute for Solid State Physics, the University of Tokyo.

-
- 1) T. M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985).
 - 2) H. Shiba, J. Phys. Soc. Jpn. **55**, 2765 (1986).
 - 3) T. M. Rice and K. Ueda, Phys. Rev. B **34**, 6420 (1986).
 - 4) P. Fazekas and B. H. Brandow, Phys. Scr. **36**, 809 (1987).
 - 5) A. M. Reynolds, D. M. Edwards, and A. C. Hewson, J. Phys.: Condens. Matter **4**, 7589 (1992).
 - 6) V. Dorin and P. Schlottmann, J. Appl. Phys. **73**, 5400 (1993).
 - 7) V. Dorin and P. Schlottmann, Phys. Rev. B **47**, 5095 (1993).
 - 8) H. Yokoyama and S. Tokizaki, Physica B **230-232**, 418 (1997).
 - 9) H. Watanabe and M. Ogata, J. Phys. Soc. Jpn. **78**, 024715 (2009).
 - 10) K. Kubo, Phys. Rev. B **87**, 195127 (2013).
 - 11) K. Kubo, J. Phys. Soc. Jpn. **84**, 094702 (2015).
 - 12) T. Okabe, J. Phys. Soc. Jpn. **66**, 2129 (1997).
 - 13) J. Bünnemann, W. Weber, and F. Gebhard, Phys. Rev. B **57**, 6896 (1998).
 - 14) K. Kobayashi and H. Yokoyama, Physica C **445-448**, 162 (2006).
 - 15) K. Kubo, Phys. Rev. B **79**, 020407(R) (2009).
 - 16) K. Kubo and P. Thalmeier, J. Phys. Soc. Jpn. **80**, SA121 (2011).
 - 17) S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
 - 18) H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987).
 - 19) H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **59**, 3669 (1990).
 - 20) C. S. Hellberg and E. J. Mele, Phys. Rev. Lett. **67**, 2080 (1991).
 - 21) N. Kawakami and P. Horsch, Phys. Rev. Lett. **68**, 3110 (1992).
 - 22) C. S. Hellberg and E. J. Mele, Phys. Rev. Lett. **68**, 3111 (1992).